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DEVELOPMENT OF THE GEM (GENERAL ELLIPTIC MARCHING)
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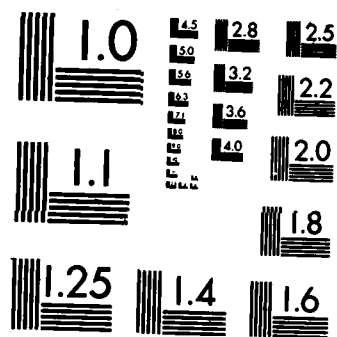


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The development and testing of the GEM (general elliptic marching) codes is described. The GEM codes solve elliptic and mixed discretized 2D pde's by direct (non-iterative) spatial marching methods, in as few as 2 SOR iterations. Both 5-point and 9-point stencils may be solved, with no requirement that the coefficients be separable, and quite general boundary conditions are allowed. Also described is the use of Symbolic Manipulation to produce Fortran coding of the 2D and 3D stencils for boundary fitted coordinate problems, and validation methods.

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DEVELOPMENT OF THE GEM PACKAGE: USER-ORIENTED
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AND MIXED PARTIAL DIFFERENTIAL EQUATIONS

Final Report 83-1

PATRICK J. ROACHE
18 February 1983

U.S. Army Research Office
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Ecodynamics Research Associates, Inc.
P. O. Box 8172
Albuquerque, New Mexico 87198

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STATEMENT OF THE PROBLEMS STUDIED

Under the initial funding of this contract, the GEM codes for the solution of two-dimensional discretized elliptic and mixed partial differential equations were developed and tested. The codes are based on spatial marching methods. Attention was directed to the non-separable problems, since the marching methods are the only practical direct method of solution for these problems. The work included development and evaluation of stabilizing methods, and options for general boundary conditions, including periodicity. The work emphasized the benchmark testing, including the penalties associated with the stabilizing methods, and comparisons with theoretical operation counts. These results and code documentation were published in the open literature, and the codes made available to the scientific community.

Under supplementary funding, Symbolic Manipulation was used to analytically transform general elliptic equations to boundary-fitted (non-orthogonal) coordinate systems, to substitute the finite difference equations, to consolidate terms, and to write a Fortran subroutine for the generation of the finite difference stencil. This stencil was then passed to a canned solver (the GEM codes in two dimensions) to solve the problem. Although the scope of the proposal only included the field equation in two dimensions, the work was actually accomplished for both the field equation and the coordinate generating equations, and for both two and three dimensions.

SUMMARY OF RESULTS

GEM CODES

A very general version of the unstabilized marching methods was coded. The code includes options for 5- and 9-point non-separable operators and general boundary conditions. In addition to the usual linear combinations of Dirichlet and Neumann boundary conditions, the code also treats combinations of tangential derivatives (important for transonic flow applications), and periodic conditions in the direction transverse to the march.

With the options for periodic boundary conditions plus the general 9-point operator, each step in the march requires a tri-diagonal solution with variable coefficients and periodic boundary conditions. A new algorithm was devised for this subproblem which is more efficient than existing algorithms (e.g. see Temperton, J. Comp. Phys., 19, 317-323, 1975) for the variable coefficient problem of interest.

The timing tests without stabilization were gratifying. The operation counts previously derived were verified. As predicted, the marching method solves repeat solutions of the 5-point operator is about the equivalent of 2 SOR iterations. (If a convergence test is included in the SOR operation, which is the practical comparison, the marching method solves the 5-point equation in a CPU time equivalent to 1.8 SOR iterations on a CDC 6600.) Nine-point problems in a 101x101 mesh have been solved. The agreement with the operation count for initialization is acceptable but not as good, with the actual timing tests being about 40% higher than predicted, depending somewhat on the problem size. Some of this discrepancy is due to the use of a condition estimator in the Gaussian elimination routine (from LINPACK) but in any case the theoretical estimate is satisfactory. This CPU time for initialization is also comparable to the multigrid results attained by A. Jameson of Courant Institute on non-separable problems. (The

option to obtain an estimate of the influence matrix condition number has proved valuable in debugging the problem description.)

A re-evaluation of the stabilizing schemes was necessitated by consideration of expanding mesh problems. Based on multiple criteria, including operation count for initialization, operation count for repeat solutions, storage penalty, size of the auxiliary matrices involved (affecting round-off error in the Gaussian elimination) and the directionality of each march, it was decided to use the multiple patching method of stabilization. This is the least elegant of the candidates. The need in many practical problems (e.g. boundary layer problems) to march the solution in only one direction eliminated the Russo-Madala scheme. The "influence extending" method previously developed by the P.I. has larger storage penalties for auxiliary matrices. (Attempts to reduce this storage penalty were unsuccessful.) The storage could be accomplished by using slow external storage, but this would make the code less transportable. The multiple marching method also has large storage penalties and severe round-off problems beyond a mesh doubling of the simple marching problem. The chosen multiple patching method has a penalty of about x2 in initiation operation count compared to the best scheme (multiple marching) but is slightly faster for repeat solutions, which is the expected primary use of the code. More importantly, it has only half the storage penalty as multiple marching for a mesh quadrupling. Also very significantly, the chosen multiple patching method allows for arbitrary marching direction in each sub-block, which would be optimum for double boundary layer problems such as asymmetric flow in a channel. The method also lends itself naturally to modular programming, in contrast to the other candidates. The already developed GEM subroutine was used, and the patching was done by a driver for the GEM subroutine.

The basic (unstabilized) GEM code had to be extended for use with the stabilizing driver based on the patching algorithm. These extensions are significant improvements in themselves, allowing the user to select the march direction, which is significant for

expanding mesh problems. Although trivial from an algorithmic point of view, this extension involved significant coding and debugging due to complex interactions with other options. Other extensions are as follows: the subroutine is CALLable with different problem specifications in the same main program; all ten matrices which define the problem are convertible to Fortran FUNCTIONS (which necessitated their removal from all argument lists at first- and lower-level calls); a segmented solution capability is available, with Dirichlet over-ride and homogeneous solution over-ride of the problem matrix specification.

The initial timing test on a two-patch solution of the 5-point operator verified the operation count predictions for repeat solutions very well, doubling the CPU time for the 0-patch (basic) code. The penalty for initialization is only a factor of 3.2, less than the predicted value of 4.3. The coding for the 4-patch driver was similar to the 2-patch driver, with CPU time for repeat solutions predicted to increase by a factor 4.3 compared to 0-patch, and initialization by ~ 10 . However, the interaction with the many options for boundary conditions made this coding quite difficult.

The stabilizing code GEMPAT2 nominally doubles the problem size in the marching direction, and GEMPAT4 nominally quadruples the problem size. The generality of the codes was demonstrated by calculation of 5-point and 9-point stencils with all the matrix elements containing a random number component, including the boundary conditions.

The stabilizing codes GEMPAT2 and GEMPAT4 nominally double and quadruple the problem size in the marching direction; however, some degradation in the accuracy was noted, apparently due to the interaction of the rounding errors from the marching method and from the solution of the patching matrix. The timing penalty for the mesh doubling and mesh quadrupling codes is reasonable for repeat solutions, but becomes a serious disadvantage for initialization as the number of patching regions increases. The rapidly

deteriorating initialization time, decreasing accuracy (compared to the nominal) and the rapidly increasing storage penalty for the patching matrices indicate that the patching algorithms become impractical beyond the 4-patch solution. The maximum problem size remains strongly dependent on a favorable cell aspect ratio.

A single corrective iteration, which increases the repeat solution time by 50% to 60%, markedly improves the accuracy of the 9-point periodic operator, and is recommended as a standard use for this problem. For other problems, the effect of the corrective iteration is somewhat unpredictable, usually giving a small increase in accuracy but sometimes giving a decrease.

Carefully performed operation counts of the algorithm were shown to be a dependable and fairly accurate indicator of the relative computational speed of the codes.

The summary article on the capabilities and the timing and accuracy tests of the GEM codes was published in Numerical Heat Transfer. A reprint of that article is included as part of this final report. Earlier versions were presented at a LASL conference and at the 1981 Army Numerical Analysis and Computers Conference, and published in those Proceedings; see lists of publications and presentations. Other presentations on the GEM codes and their use in semidirect nonlinear solution procedures were given at Ohio State University, at the Symposium on Numerical and Physical Aspects of Aerodynamics Flows, at NASA-Lewis Research Center, at the 3rd IEEE International Pulsed Power Conference, at Mississippi State University, at C.N.R. in Rome, and at the IAHR Workshop held in Rome.

Extensive experience was gained using the GEM codes in grid generation problems using elliptic generating equations. GEM is particularly well suited to these problems, because the two generating equations both have the same solution matrix (thus requiring only one GEM initialization), and because the coordinate transformation procedure often produces the desired cell aspect

ratio important to the stability of the marching methods. Initial applications were presented at the 3rd IEEE International Pulsed Power Conference in 1981 and published in the Proceedings. An invited paper on these applications, entitled "Interactive Design of Laser Electrodes Using Elliptic Grid Generation and Semidirect/Marching Methods" was presented at the Army Numerical Analysis and Computers Conference held 3-4 February 1982 in Vicksburg, Mississippi and published in the Proceedings. Also, a contributed paper entitled "Semidirect/Marching Solutions and Elliptic Grid Generation" was presented at the Symposium on Numerical Grid Generation for Numerical Solutions of Partial Differential Equations held 13-16 April 1982 at Nashville, Tennessee, and published by North-Holland in the Proceedings.

The marching methods were applied in a semidirect solution of separated flow in non-orthogonal coordinates, and several aspects of the algorithm emerged in this study. Three-point $O(\Delta^2)$ accurate gradient boundary conditions were coded directly into the marching method; for the 9-point operator, this increased the band width of the tridiagonal marching equation. This was treated by special Gaussian elimination at the near-boundary points. This treatment was satisfactory for the transformed Poisson equation, but for the vorticity equation at high Reynolds number (in which the corner terms of the 9-point matrix become very small) a deteriorating condition of the marching matrix resulted in large round-off errors in the fine (81x81) mesh. The problem was solved by using only 2-point $O(\Delta)$ gradient conditions in the direct marching algorithm, with the 3-point correction to $O(\Delta^2)$ accuracy being lagged in the nonlinear iterations. This procedure converged very quickly and is more robust than the direct 3-point method. Consequently, only the 2-point normal gradient formulation is allowed in the final GEM code. Also, this study demonstrated the use of the marching method in a systematically refined grid (11x11 to 81x81) with a 9-point operator, and demonstrated that the very small residual errors of the marching method allows Richardson extrapolation to be used on the non-orthogonal mesh

to achieve $O(\Delta^4)$ accurate solutions. A paper on this work, entitled "Scaling of High Reynolds Number Weakly Separated Flows" was presented at the Symposium of Numerical and Physical Aspects of Aerodynamic Flows" held at California State University at Long Beach, 19-21 January 1981, and published by Springer-Verlag in the Proceedings.

SYMBOLIC MANIPULATION

Once a general software package or code is chosen for the solution of the matrix problem, the remaining problem for the user is still formidable; that is, the problem of formulating the matrix problem from the physical problem. This is a tedious and error-prone procedure. The supplemental funding on this contract addressed this problem by way of computer Symbolic Manipulation.

The Symbolic Manipulation work was especially successful. The primary objective was achieved early with a demonstration and verification of the procedure in two dimensions. The test case was changed from that in the proposal (flow in a channel) to a nonlinear electric field problem, which had the advantage of being a single equation and of already being set up (under separate funding) for the elliptic grid generation problem. The Symbolic Manipulation code Macsyma was used on the Vax computer (vaxima) at the University of New Mexico. Using vaxima, symbolic code was written first to analytically transform a variable-coefficient elliptic equation from cartesian to general (non-orthogonal) coordinates, then to substitute finite difference expressions for the partial derivatives, to consolidate terms, and finally to actually write a Fortran subroutine to generate the numerical coefficient arrays for the discretized partial differential equations. In this 2D case, the coefficients were validated by comparison with the previously developed code, which took months to debug and validate. A paper on this 2D work, entitled "Symbolic Manipulation and Computational Fluid Dynamics", was presented at the SIAM

30th Anniversary Meeting held at Stanford 19-23 July 1982. A similar early presentation was made at a seminar to the Faculty of Engineering at the University of Rome.

The Symbolic Manipulation work was then extended to three dimensions and to the grid generation problem. In the 2D case, the coefficients were validated by comparison with output from a previously developed hand-coded subroutine. For the 3D case, we developed a validation procedure which does not depend on hand-coding of a parallel solution.

The validation procedure consisted of testing the truncation-error convergence of the solution of the matrix problem. An inverse procedure was devised, in which the continuum solution was specified, chosen so as to possess enough structure to exercise all the derivatives of the operator and all the finite-difference errors. For the second-order operator and second-order accurate finite difference forms, the solution was specified as $\text{sol} = x^3y^4z^5$. The transformation used involved the hyperbolic tangent of all three transformed coordinates. The equation in the original cartesian coordinates was $L(\phi) = \nabla \cdot \sigma \nabla \phi = q$, where σ involved the sin of all three coordinates, and the non-homogeneous part q was chosen so as to give the desired solution, i.e. $q = L(\text{sol})$. This highly structured problem is then fed to the Symbolic Manipulation code, and the matrix problem generated by it is solved numerically. (In 2D, we used the GEM codes, and in 3D, we used a hopscotch SOR solver.) By monitoring the truncation error as the grid is refined from 5^3 , 9^3 , 17^3 , 33^3 , we verify the transformation, the finite difference forms (validating $O(\Delta)^2$ accuracy) and the iterative solution procedure. As predicted theoretically, the value of $C = \Delta^2 \cdot \text{TE}$, where TE is the maximum truncation error in the mesh, becomes constant as the mesh is refined. The size of C depends on the grid stretching parameters, being larger for large inappropriate stretching, but the entire method remains $O(\Delta)^2$ accurate. (This is an important demonstration in itself.)

The experience gained with the Symbolic Manipulation procedures was valuable, and resulted in significant increases in efficiency. The 3D code still requires on the order of 1 hour of cpu time on the Vax 780 to generate the matrix, but this is down more than an order of magnitude from the original version (which was also correct, but gave longer code). Some additional gain accrued when we made use of symmetries in the 19-point 3D stencil. (We did not retain the conservation form of the operator.) The 2D code is much faster, by an order of magnitude.

Our present work has had some influence on the fundamental work on Symbolic Manipulation. The Macsyma "code" is not a coherent development, but is a collection of independently developed sub-units. The whole work represents over 100 man-years of effort. It was not funded or organized as a unified project, and the resulting code has shortcomings because of this history. Recently, Richard Fateman at U. Cal. Berkeley has received funding from the Science Development Foundation to develop a new generation of Symbolic Manipulation code, based on a Macsyma that is re-built from "the ground up". Dr. Steinberg recently spent two weeks with Fateman, and will continue to work with him in this far-reaching project. Our experience is currently playing an important role in the design considerations for this new Symbolic Manipulation code, and will continue to do so. (Steinberg had significant and specific recommendations about things that Macsyma did not handle well, and in fact had developed special techniques for these PDE problems.)

At the ARO-GE Workshop on Symbolic Manipulation, held at the General Electric Corporate Research and Development Center in Schenectady, New York on 14-16 December 1982, we presented two papers on this Symbolic Manipulation work: "Symbolic Manipulation for Generation of Fortran Codes for Partial Differential Equations" by S. Steinberg, and "Numerical Aspects and Potential of Symbolic Manipulations for Partial Differential Equations" by P. J. Roache. Tutorial presentations were also given in seminars to the Faculty of Engineering at the University of Rome, and to the Department

of Mathematical Science at Rensselaer Polytechnic Institute; see list of presentations. We will also present two papers at the AIAA 6th Computational Fluid Dynamics Conference to be held 13-15 July 1983 in the Boston area. The first is an invited paper entitled "Symbolic Manipulation and Computational Fluid Dynamics", and the second is a contributed paper entitled "Validation of Three Dimensional Boundary Fitted Coordinate Codes". A Summary article on this work entitled "Symbolic Manipulation and Computational Fluid Dynamics", is in the final stage of editing and will be submitted shortly to the Journal of Computational Physics.

In future work, we intend to develop the procedure for more difficult boundary conditions. Other research areas include conditional differencing (e.g. upwind tests), conservative forms, multiequations, time dependent equations, directional splitting, higher order continuum equations, deferred corrections, and code optimization. Areas of application include coordinate transformations, finite element method development, and especially constitutive equation testing in areas such as turbulence, non-Newtonian fluids, soil mechanics, gravitational theory, high Re flow in porous media (beyond the Darcy Law regime), fingering in porous media flow, etc. Also, Dr. Steinberg will continue to consult with R. Fateman at U. Cal. Berkeley on the development of a new generation of Symbolic Manipulation code.

TECHNOLOGICAL APPLICATION

An application was made of the methods developed under this contract to a U.S. Army technological problem, in the area of Pulsed CO₂ laser development. Under separate funding from the USAF-AFWL, the GEM code developed under the present ARO contract has been applied within semidirect nonlinear iterations to very rapidly solve for the electric field and energy deposition in the cavity of an electron-beam laser and to generate a boundary-fitted coordinate system. These codes were then used in calculations of the electric field in pulsed CO₂ electron beam lasers for Joe C. Walters of the U.S. Army Redstone Arsenal. The objective was to produce a design tool which would allow the laser researcher to perturb design parameters such as electrode shape, operating characteristics such as voltage and position of the electron beam, etc. and obtain graphical display of the solution, especially the energy deposition, in a time-sharing interactive environment. The designer would perturb the parameters, looking especially for near-uniform energy deposition so as to prevent arcing in the cavity, allowing higher power levels of operation. The work has been successful on minimal funding, due in large part to the technology developed through basic research funding at ARO; not only the GEM code on the present contract, but also the semidirect nonlinear solution methods from a previous ARO contract.

LIST OF PUBLICATIONS

Roache, P. J., "GEM Solutions of Elliptic and Mixed Problems with Non-Separable 5- and 9-point Operators", Proc. LASL Conference on Elliptic Solvers, 30 June - 2 July 1980. Santa Fe, N.M., Academic Press, M. Schultz, ed., 1981, pp. 399-403.

Roache, P. J., "Scaling of High Reynolds Number Weakly Separated Channel Flows", Proc. Symposium on Numerical and Physical Aspects of Aerodynamic Flows, California State University at Long Beach, 19-21 January 1981. Springer-Verlag, T. Cebeci, Ed., pp. 87-98.

Roache, P. J., "The GEM Code: Direct Solutions of Elliptic and Mixed Problems with Non-Separable 5- and 9-Point Operators", Proc. 1981 Army Numerical Analysis and Computers Conference, Huntsville, Alabama, 26-27 February 1981.

Roache, P. J., Moeny, W. M. and Filcoff, J. A., "Computational Solutions in Body-Fitted Coordinates of Electric Fields in Externally Sustained Discharges", Proc. 3rd IEEE International Pulsed Power Conference, Albuquerque, N.M., 1-3 June 1981.

Roache, P. J., "Performance of the GEM Codes on Non-Separable 5- and 9-Point Operators", Numerical Heat Transfer, Vol. 4, No. 4, 1981, pp. 395-408.

Roache, P. J., "Interactive Design of Laser Electrodes Using Elliptic Grid Generation and Semidirect/Marching Methods", Proc. 1982 Army Numerical Analysis and Computers Conference.

Roache, P. J., "Semidirect/Marching Methods and Elliptic Grid Generation", Proc. Symposium on the Numerical Generation of Curvilinear Coordinate Systems and use in the Numerical Solution of Partial Differential Equations, April 1982, Nashville, Tenn., J. F. Thompson, ed., North-Holland, Amsterdam, pp. 729-737.

Roache, P. J. and Steinberg, S., "Symbolic Manipulation and Computational Fluid Dynamics", to be submitted to J. Computational Physics.

Roache, P. J., "Validation of Three Dimensional Boundary Fitted Coordinate Codes", to be submitted to AIAA Journal.

Steinberg, S., "Change of Variables in Partial Differential Equations", to be submitted to ACM SigSam Bulletin.

LIST OF PRESENTATIONS

"Semidirect Methods in Fluid Dynamics", Boyd Lecturship, College of Engineering, Ohio State University, 5 March 1980.

"GEM Solutions of Elliptic and Mixed Problems with Non-Separable 5- and 9-Point Operators", LASL Conference on Elliptic Solvers, Santa Fe, N.M., 30 June - 2 July 1980.

"Scaling of High Reynolds Number Weakly Separated Channel Flows", Symposium on Numerical and Physical Aspects of Aerodynamic Flows, California State University at Long Beach, 19-21 January 1981.

"The GEM Code: Direct Solutions of Elliptic and Mixed Problems with Non-Separable 5- and 9-Point Operators", 1981 Army Numerical Analysis and Computers Conference, Huntsville, Alabama, 26-27 February 1981.

"Computational Fluid Dynamics Using Semidirect Methods", NASA-Lewis Research Center, 27 March 1981.

"Computational Solutions in Body-Fitted Coordinates of Electric Fields in Externally Sustained Discharges", with W. M. Moeny and J. A. Filcoff, Proc. 3rd IEEE International Pulsed Power Conference, Albuquerque, N. M., 1-3 June 1981.

"Interactive Design of Laser Electrodes Using Elliptic Grid Generation and Semidirect/Marching Methods", 1982 Army Numerical Analysis and Computers Conference, Waterways Experiment Station, Vicksburg, Miss., 3-4 February 1982.

"Solution of Elliptic Equations with the GEM Codes", Mississippi State University, Dept. of Aerospace Engineering, 5 February 1982.

"Semidirect/Marching Methods and Elliptic Grid Generation", Symposium on the Numerical Generation of Curvilinear Coordinate Systems and Use in the Numerical Solution of Partial Differential Equations, April 1982, Nashville, Tenn.

"Marching Methods for Elliptic Equations: The GEM Codes", C.N.R., Rome, Italy, 23 June 1982.

"Semidirect Methods in Fluid Dynamics", C.N.R., Rome, Italy, 23 June 1982.

"Benchmark Solution for the Expanding Channel Problem", IAHR Workshop, Rome, Italy, 24 June 1982.

"Symbolic Manipulation and Computational Fluid Dynamics", Seminaria de Faculta di Ingeneria, Univ. Roma, Rome, Italy, 26 June 1982.

"Symbolic Manipulation and Computational Fluid Dynamics", SIAM 30th Anniversary Meeting, Stanford University, 19-23 July 1982.

"Symbolic Manipulation for Generation of Fortran Codes for Partial Differential Equations", Army Research Office - General Electric Workshop on Symbolic Computations, General Electric Research and Development Center, Schenectady, New York, 14 December 1982.

"Numerical Aspects and Potential of Symbolic Manipulations for Partial Differential Equations", Army Research Office - General Electric Workshop on Symbolic Computations, General Electric Research and Development Center, Schenectady, New York, 14 December 1982.

"Symbolic Manipulation and Computational Fluid Dynamics", Large Scale Computation Colloquium, Department of Mathematical Sciences, Rensselaer Polytechnic Institute, Troy, New York, 13 December 1982.

"Symbolic Manipulation and Computational Fluid Dynamics", Invited Paper, AIAA Sixth Computational Fluid Dynamics Conference, Danvers, Mass., 13-15 July 1983.

"Validation of Three Dimensional Boundary Fitted Coordinate Codes", AIAA Sixth Computational Fluid Dynamics Conference, Danvers, Mass., 13-15 July 1983.

LIST OF SCIENTIFIC PERSONNEL SUPPORTED

Patrick J. Roache, Stanly Steinberg

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